Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-

1546-95-8 | DTXSID70165670

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 962 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.40e-01

Confidence level: 6.45e-01

Nearest Neighbors from the Training Set

Image not found
Chlorthal-dimethyl
Measured: 5010
Predicted: 2160

Image not found
Benodanil
Measured: 661
Predicted: 828

Image not found
2-(2,4,5-Trichlorophenoxy)propionic acid
Measured: 56.2
Predicted: 122

Image not found
Fthalide
Measured: 2000
Predicted: 1600

Image not found
Tetrachlorophthalic acid
Measured: 2000
Predicted: 1980